Derivative-free optimization of composite functions

Jeffrey Larson

Argonne National Laboratory

May 27, 2019

Problem setup

$$\underset{x}{\text{minimize}}\ f(x) = h(x; S(x))$$
$$\text{subject to: } x \in \mathcal{D} \subset \mathbb{R}^n$$

where the objective f depends on the output(s) from a simulation S and a known function h.

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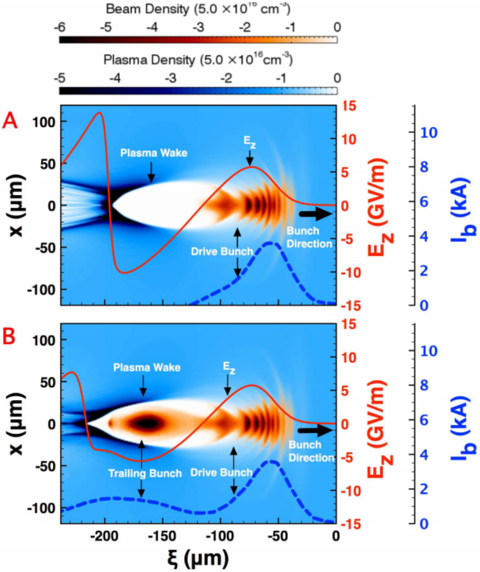
where the objective f depends on the output(s) from a simulation S and a known function h.

- Derivatives of S may not be available
- Constraints defining $\mathcal{D}$ may or may not depend on S
- The dimension n is small
- Evaluating S is expensive (not using grids or randomized/evolutionary methods)

Computers/Simulations!



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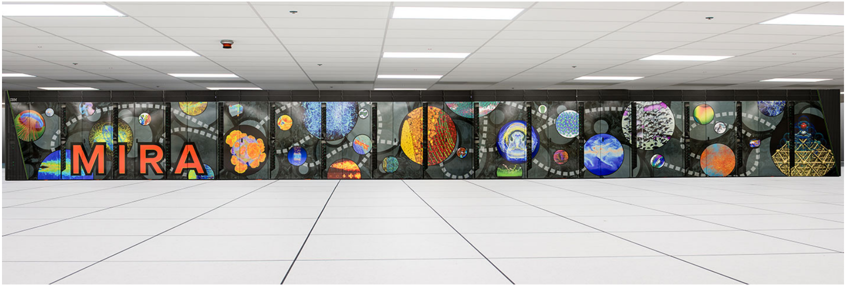
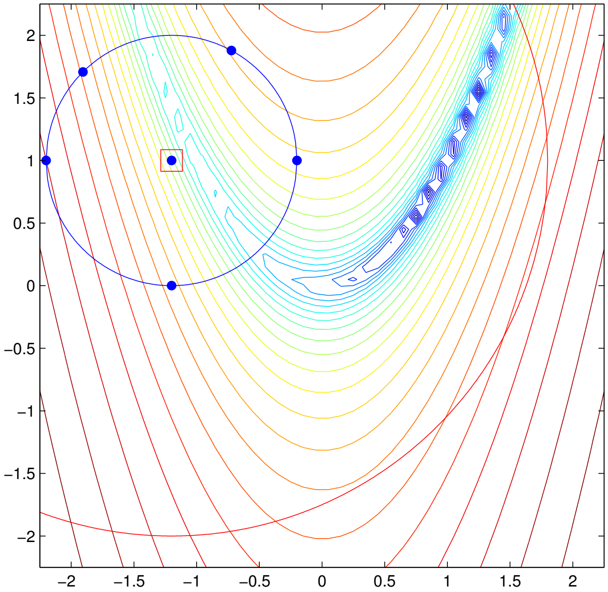


#21 on TOP500 November 2018 (#6 on TOP500 June 2016)

Model-based methods - Interpolation



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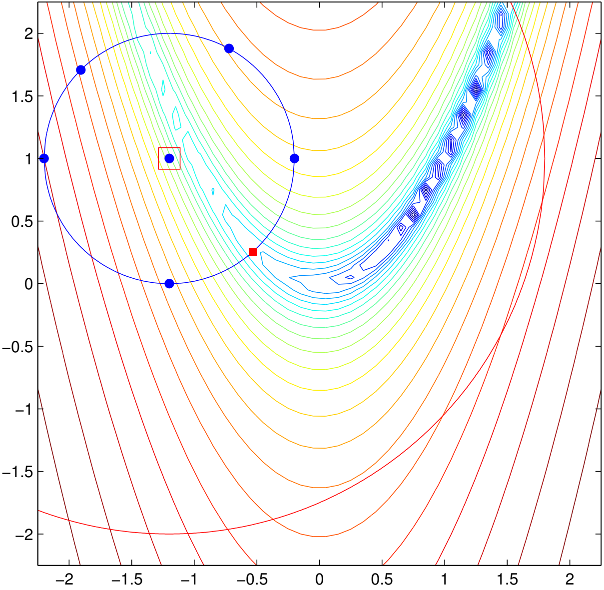

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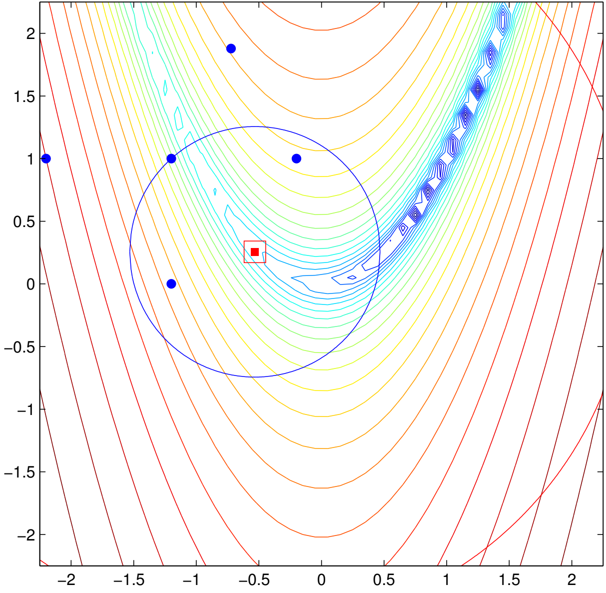

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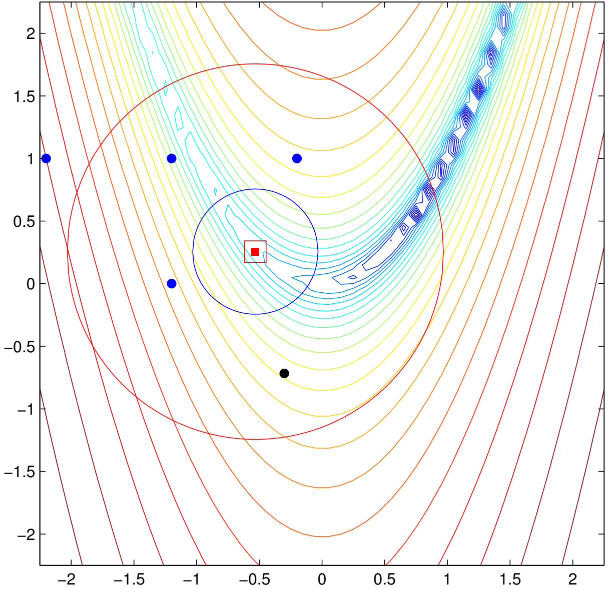

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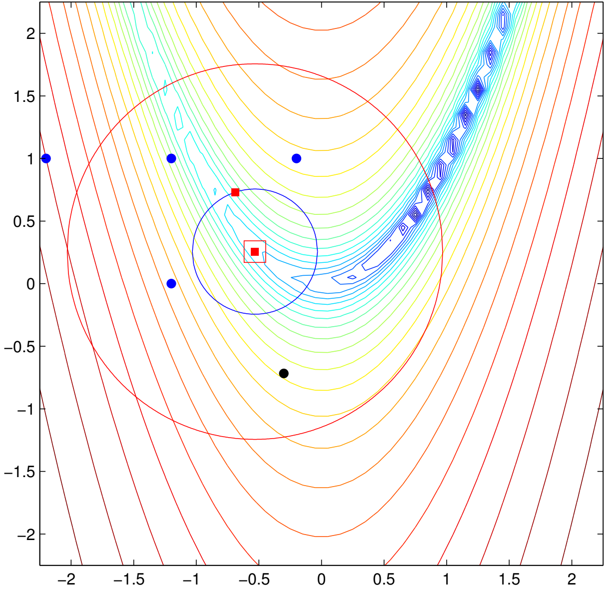

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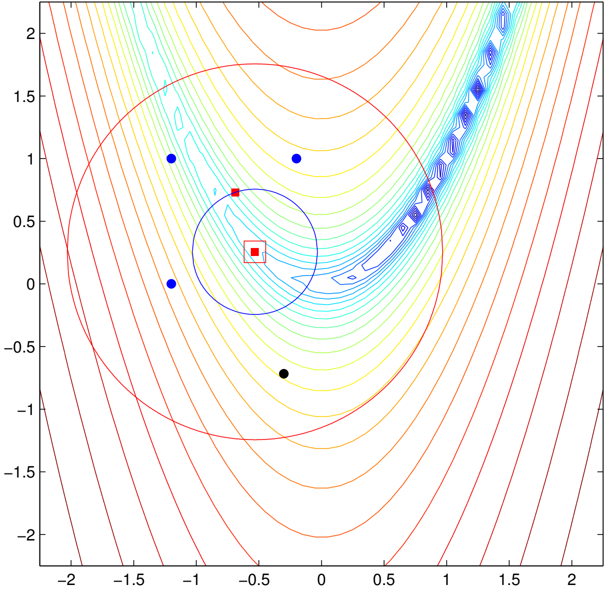

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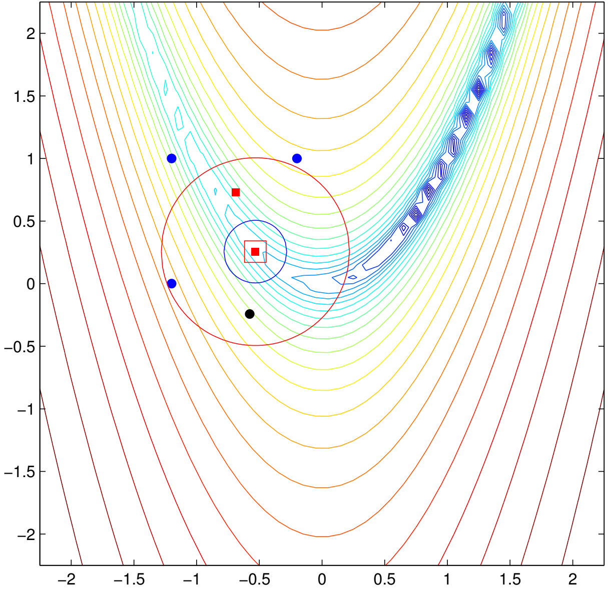

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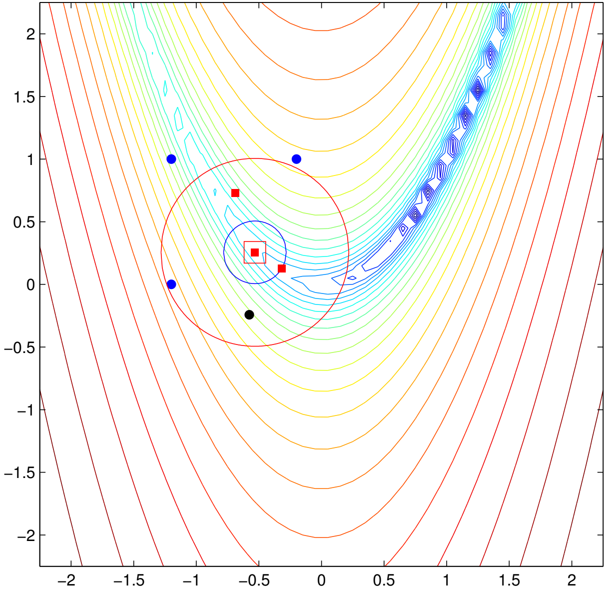

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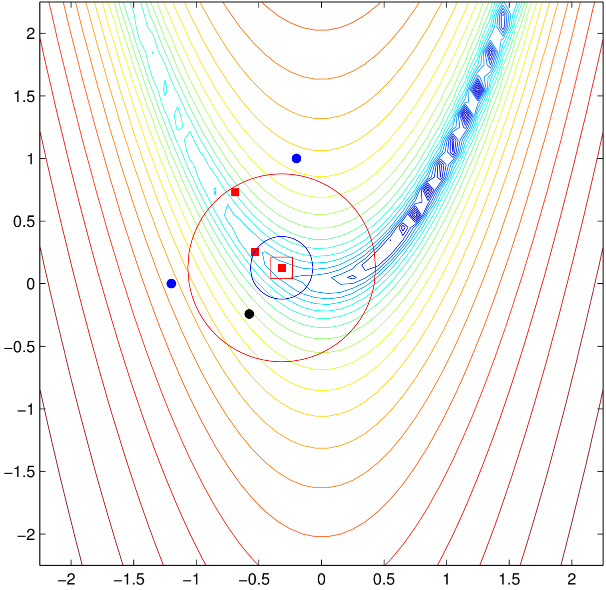

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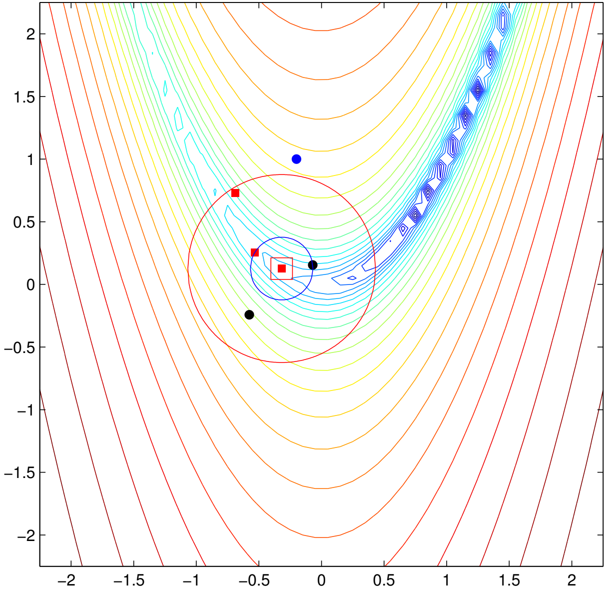

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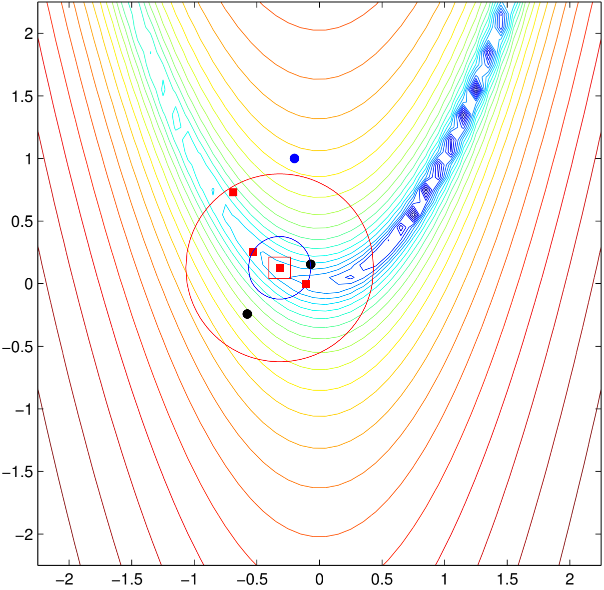

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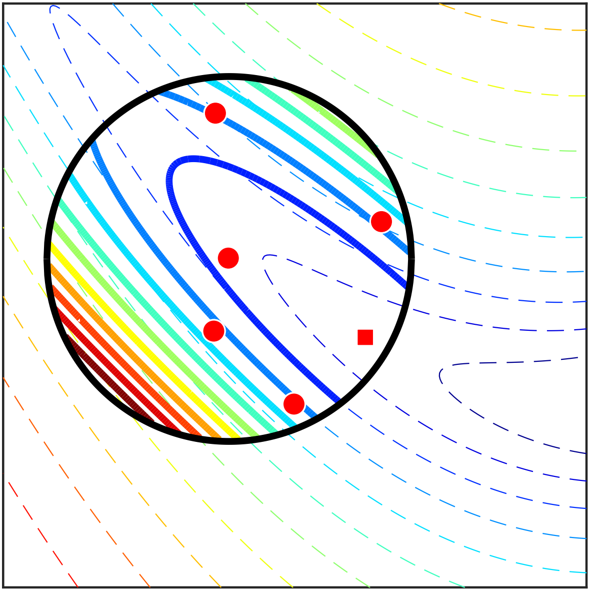

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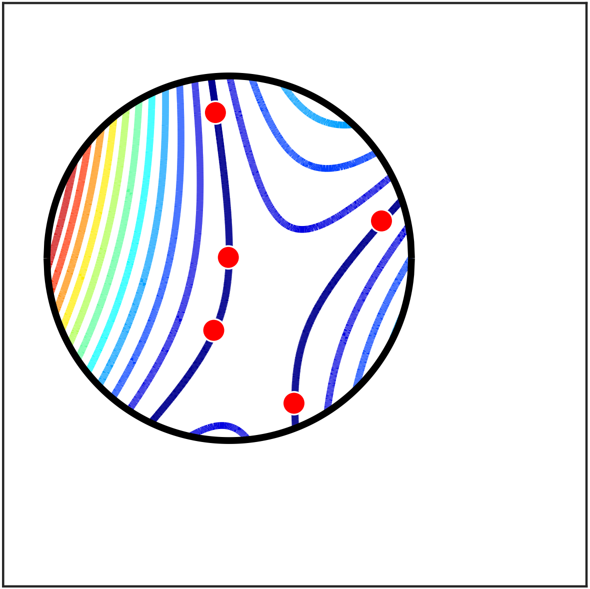

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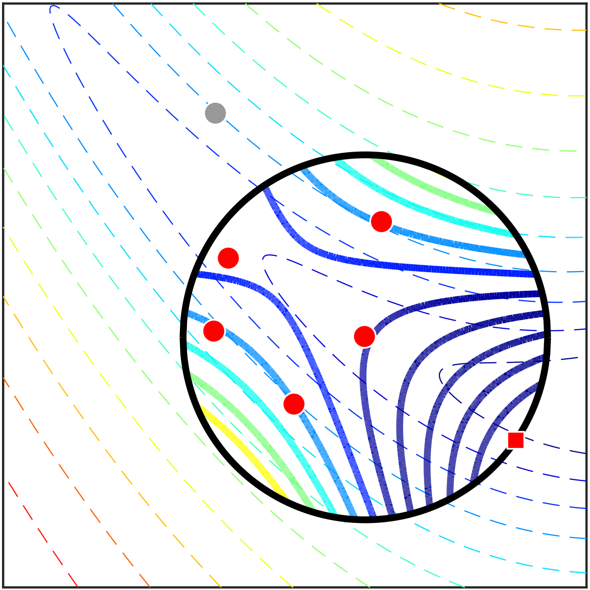

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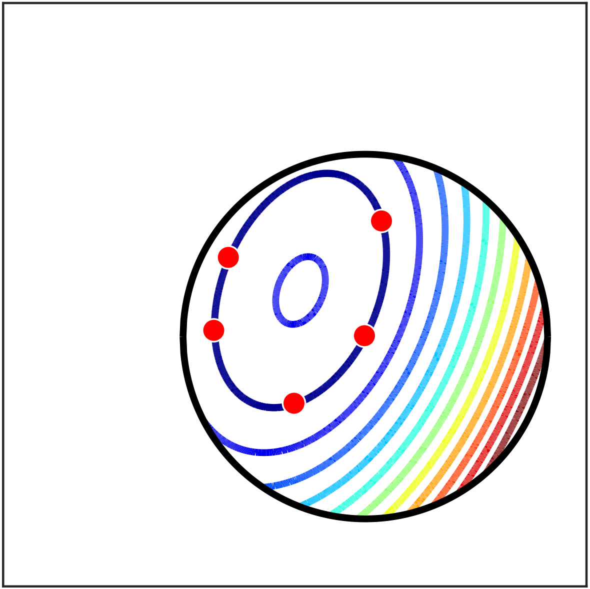

Opening up the black box

$$f(x) = \|S(x) - T\|_2^2 = \sum_{i=1}^{p}(S_i(x) - T_i)^2$$

Can either have a solver that uses $f(x)$ or $[S_1(x), \ldots, S_p(x)]$.

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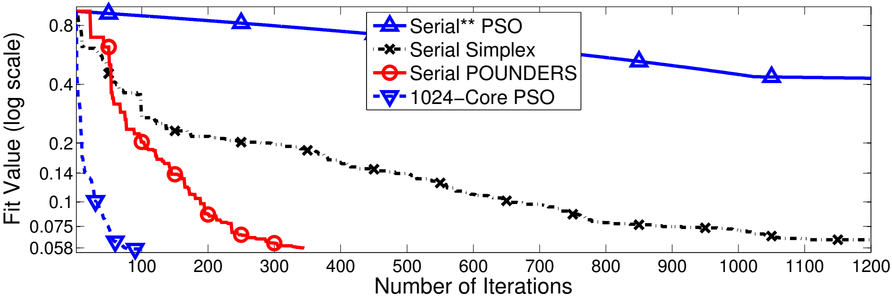

Tuning quadrupole moments for a particle accelerator simulation.

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Emittance minimization

$$\underset{v \in \mathbb{R}^n}{\text{minimize}}\ \epsilon(v)$$

$$\textbf{subject to: } v \in \mathcal{D}$$

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$$\epsilon(v) = \sqrt{\langle x(v)^2 \rangle \langle p_x(v)^2 \rangle - \langle x p_x(v) \rangle^2}$$

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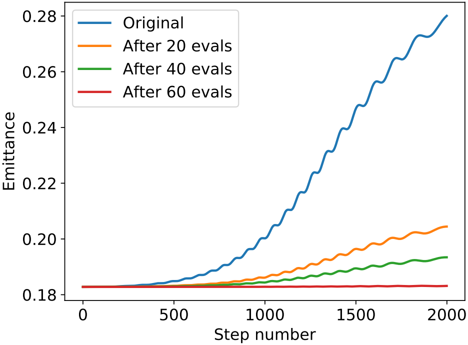

Emittance minimization

$$\underset{v \in \mathbb{R}^n}{\text{minimize}} \ \min_t \epsilon(v, t)$$

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$$0 \leq t \leq \bar{t},$$

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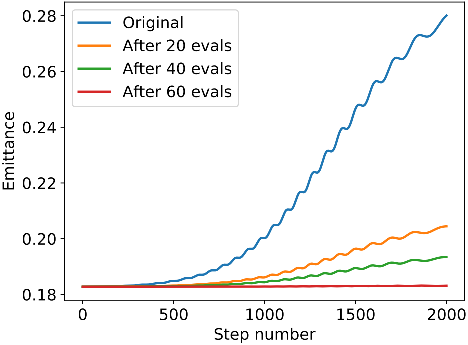


Exploiting Structure

- Nonsmooth, composite optimization

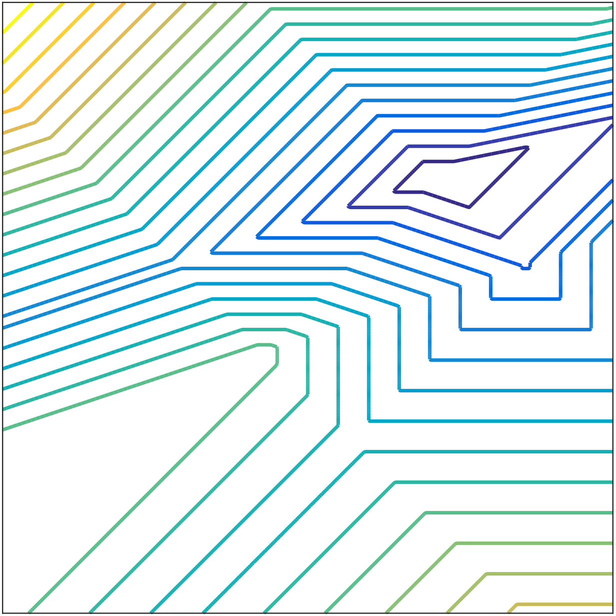
$$\underset{x}{\text{minimize}}\, f(x) = h(S(x))$$

nonsmooth $h\colon \mathbb{R}^p \to \mathbb{R}$ (with a known structure), smooth $S\colon \mathbb{R}^n \to \mathbb{R}^p$ (expensive to evaluate).

- Idea: Build p models, one for each component of S. Use model gradients in place of ∇S.
- Requires a *manifold representation* of h.
- Example: censored ℓ_1 loss:

$$f(x) = \sum_{i=1}^{p} |d_i - \max\{c_i, S_i(x)\}|$$

Censored ℓ_1 loss



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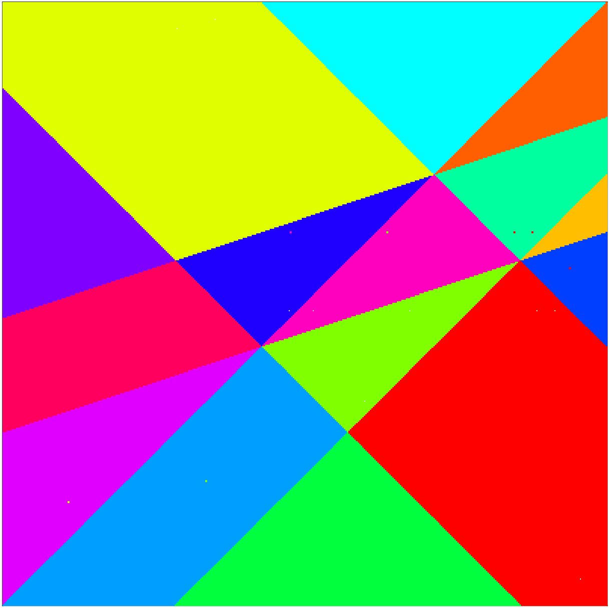

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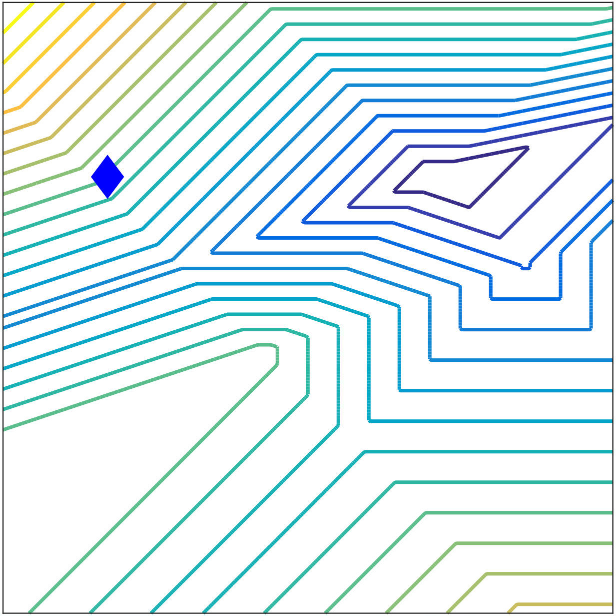
User scripts need to calculate:

$f(x)$, $S(x)$, $\mathbb{H}(S(x))$, $\{\nabla h_i(S(x)) : i \in \mathbb{H}(S(x))\}$, $\{h_i(S(x)) : i \in \mathbb{G}\}$,

Manifold Sampling



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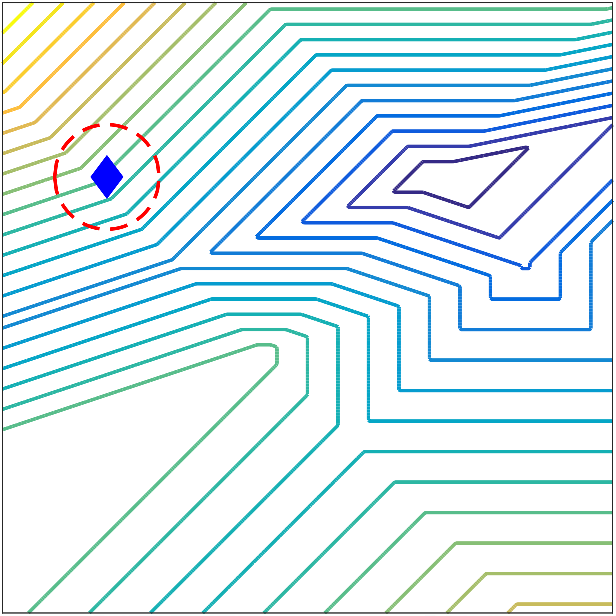

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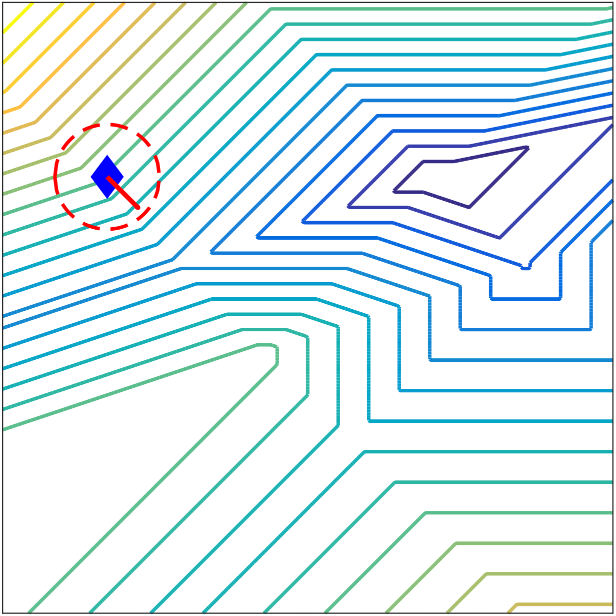

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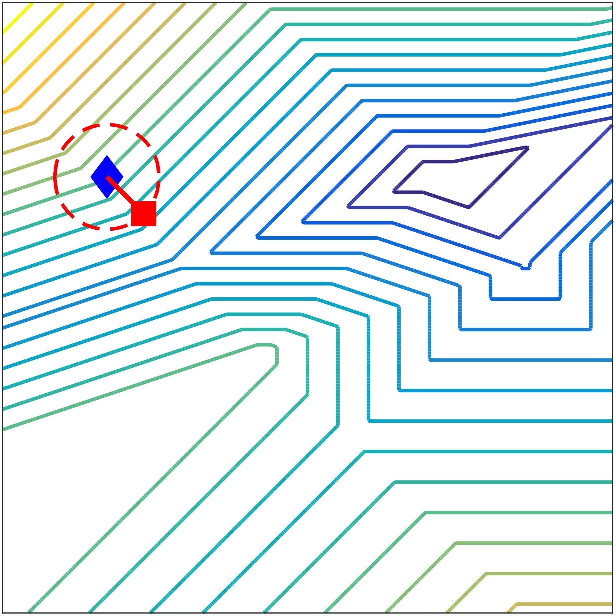

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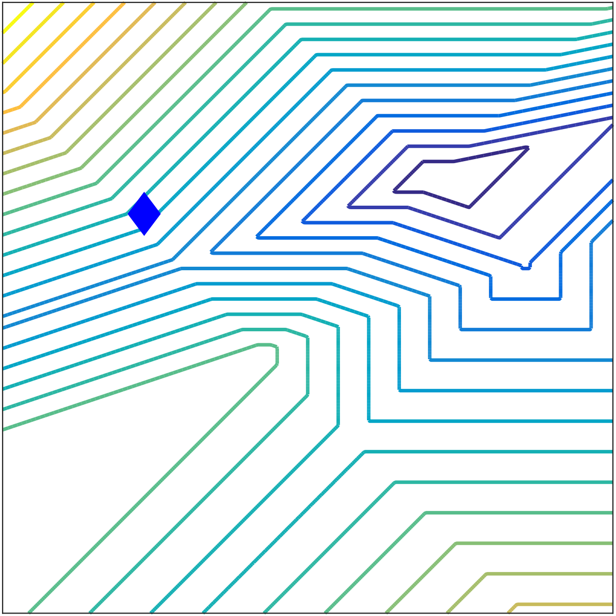

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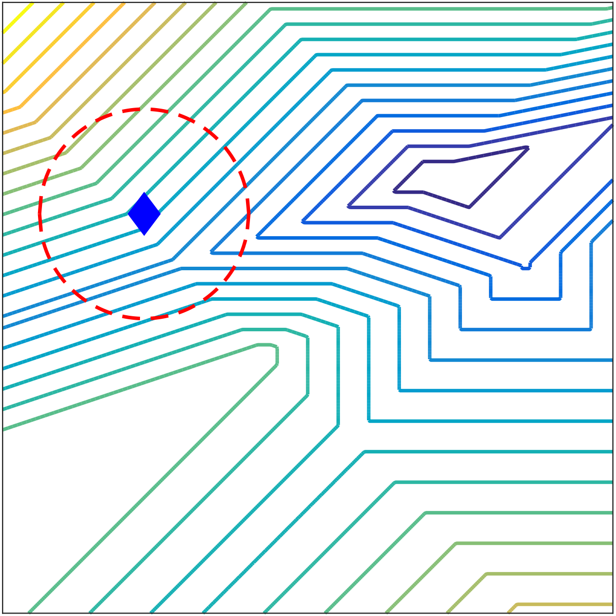

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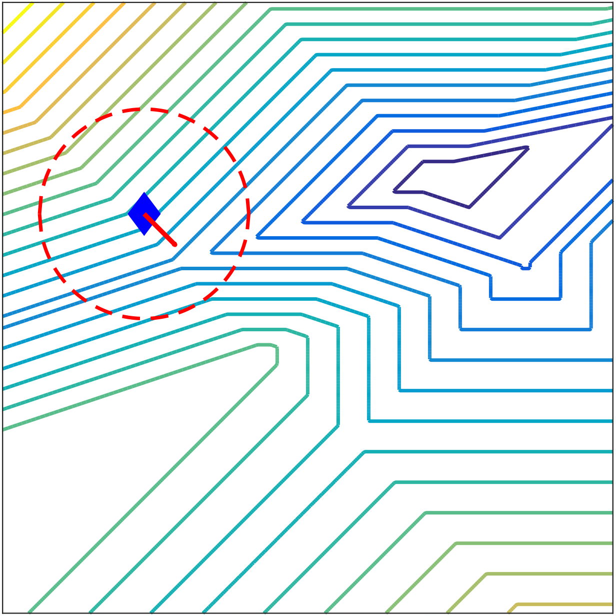

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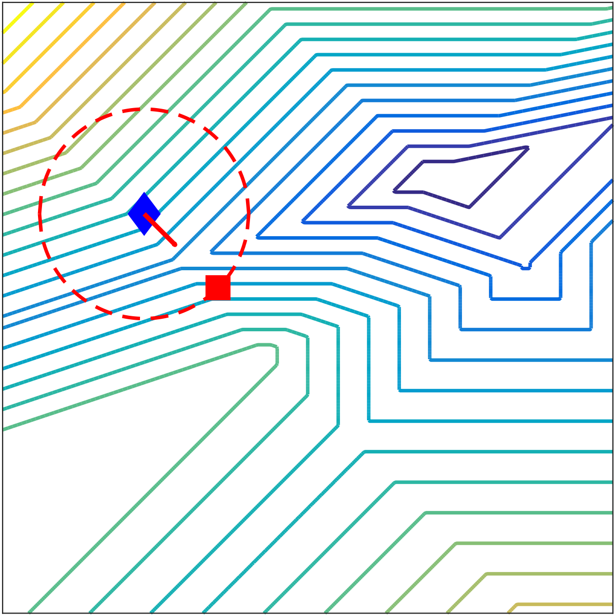

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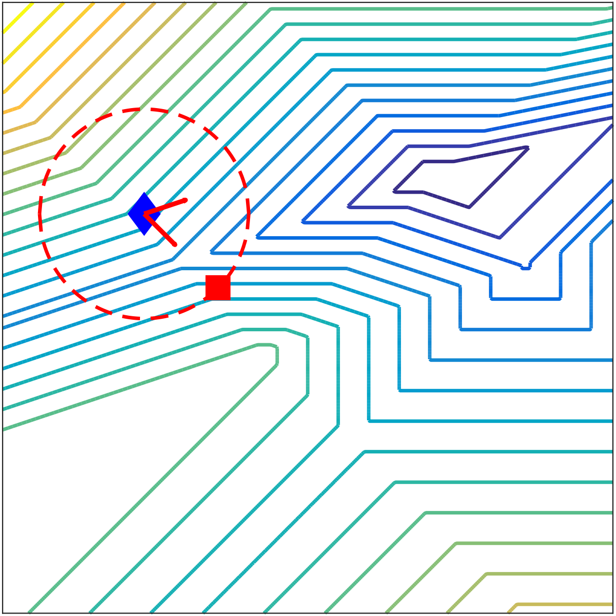

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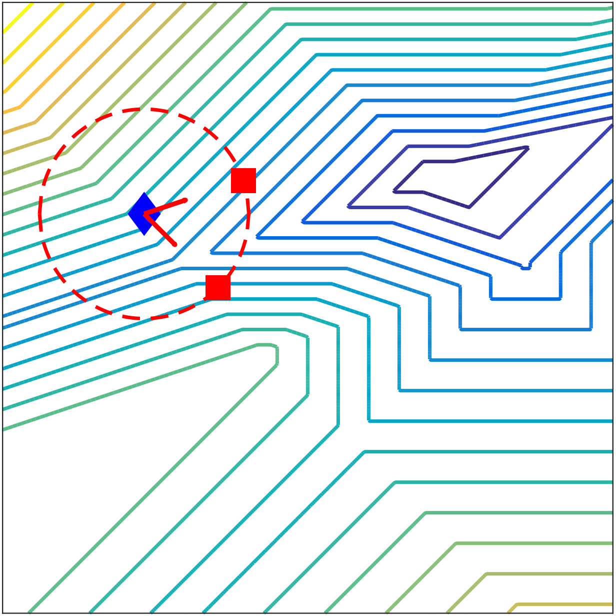

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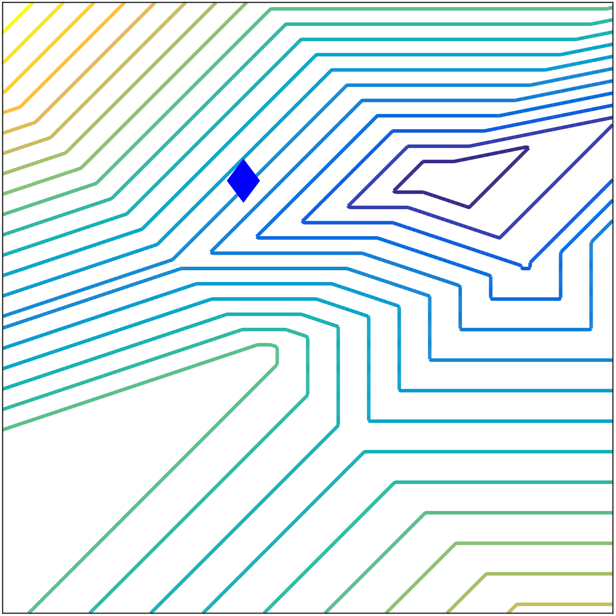

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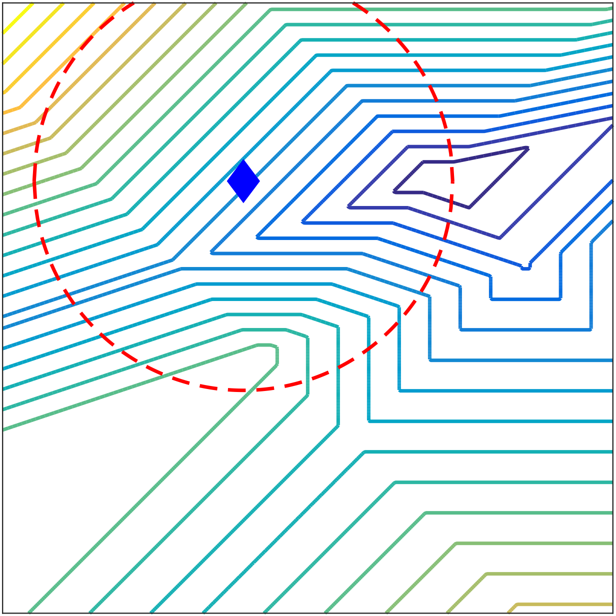

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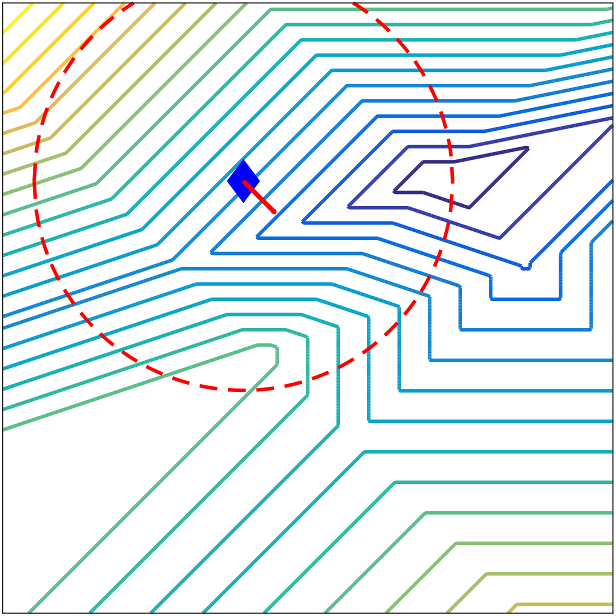

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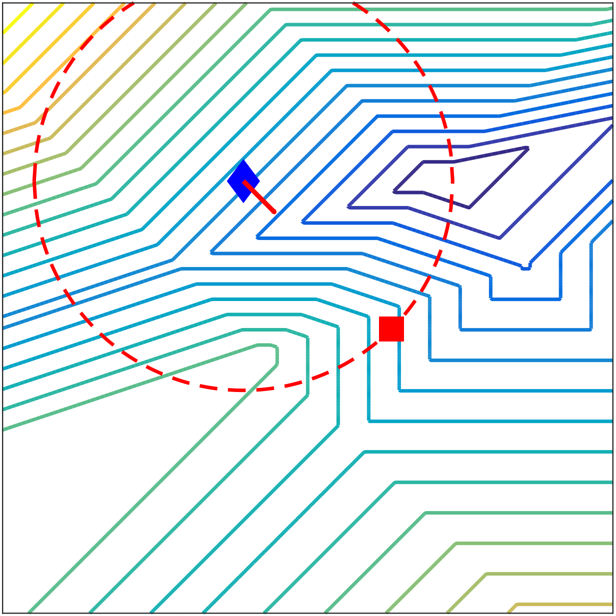

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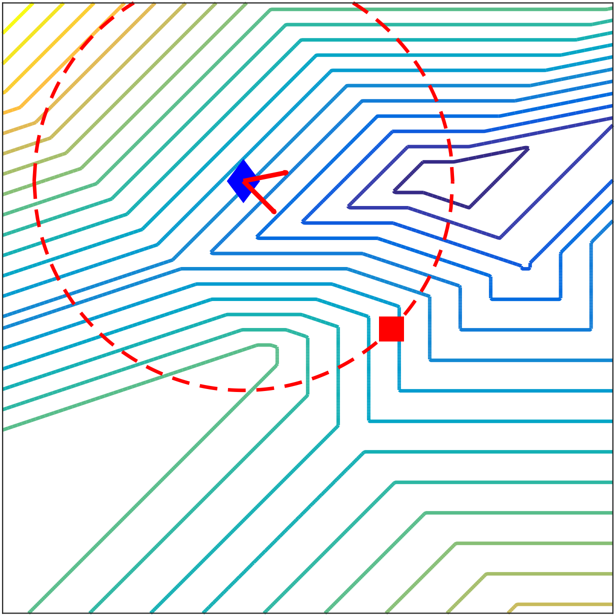

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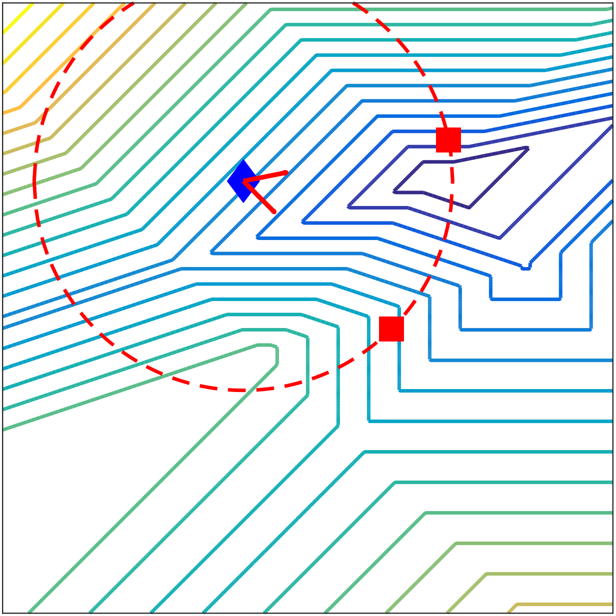

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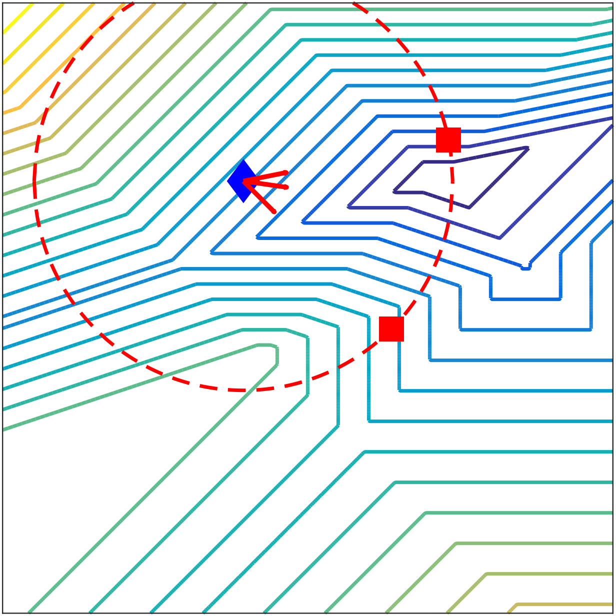

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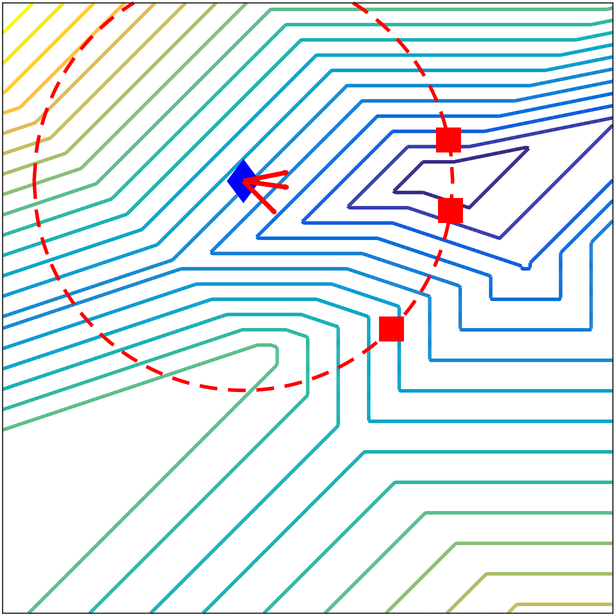

Smooth master model

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Define the smooth *master model* $m_k^f : \mathbb{R}^n \to \mathbb{R}$ (with gradient g^k) and obtain step by (approximately) solving

$$\underset{s}{\text{minimize}}\; m_k^f(x^k + s)$$

$$\text{subject to: } s \in \mathcal{B}(0, \Delta_k)$$

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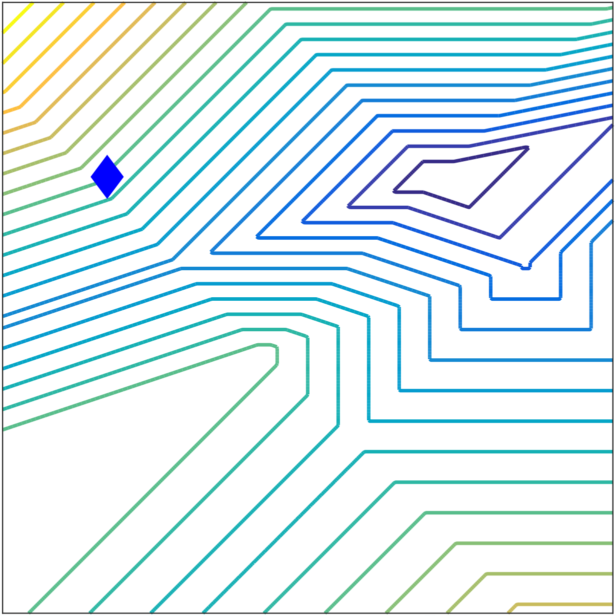

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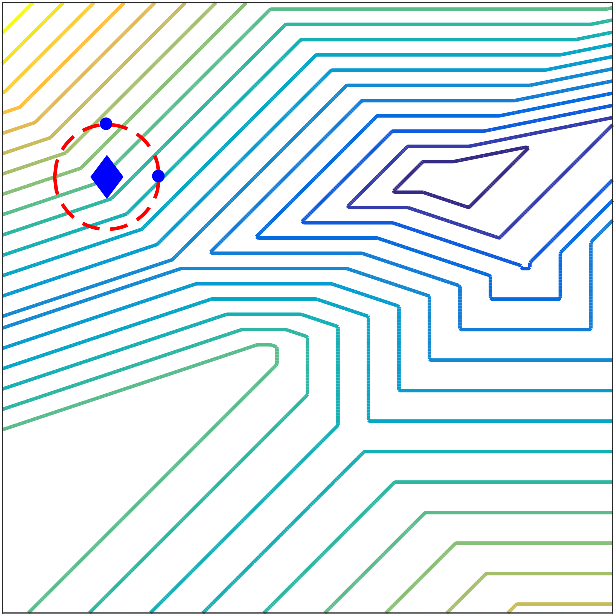

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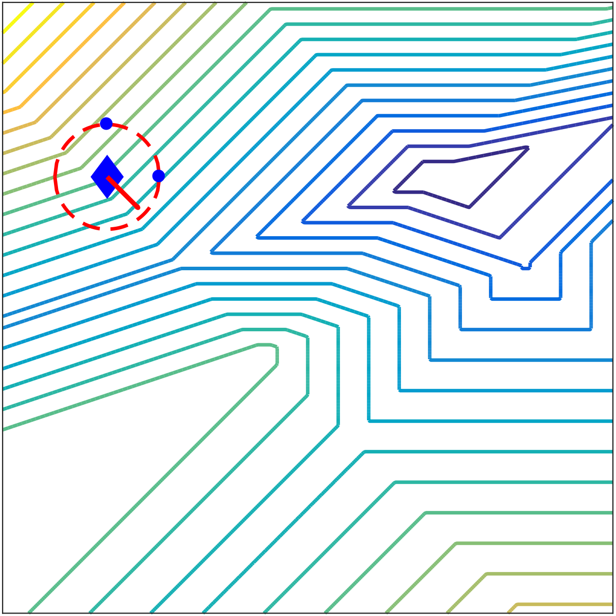

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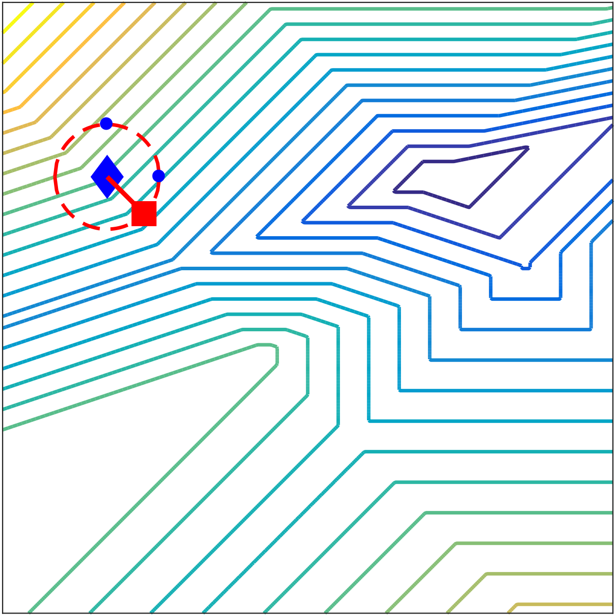

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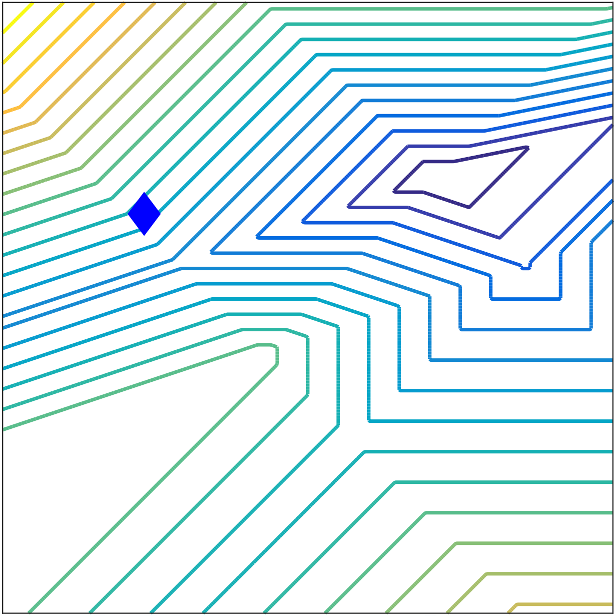

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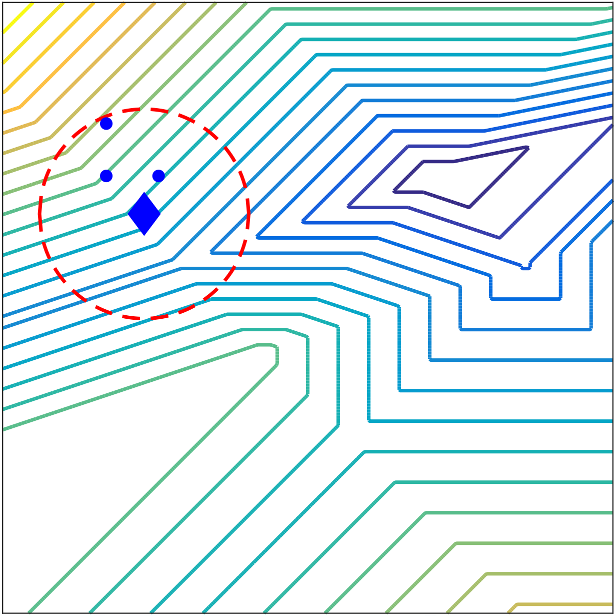

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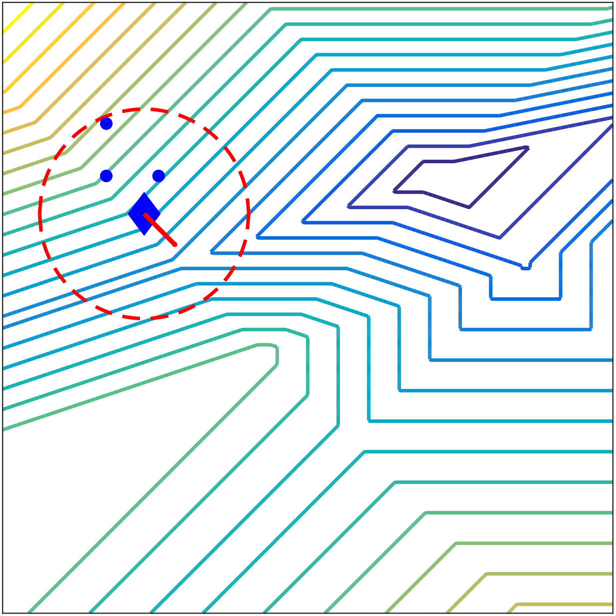

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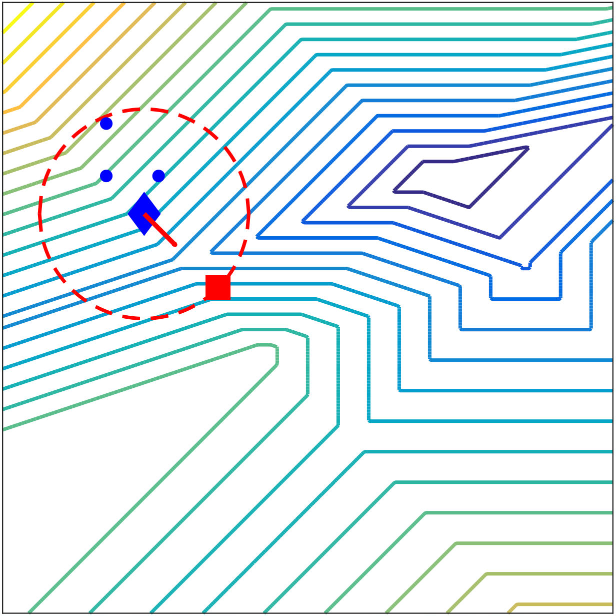

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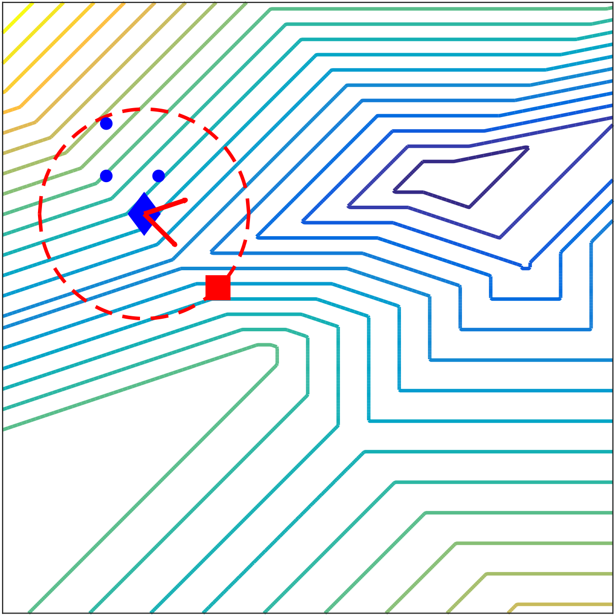

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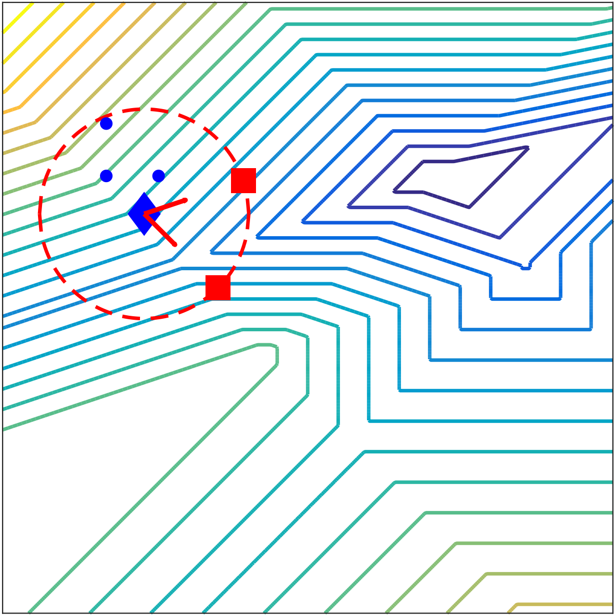

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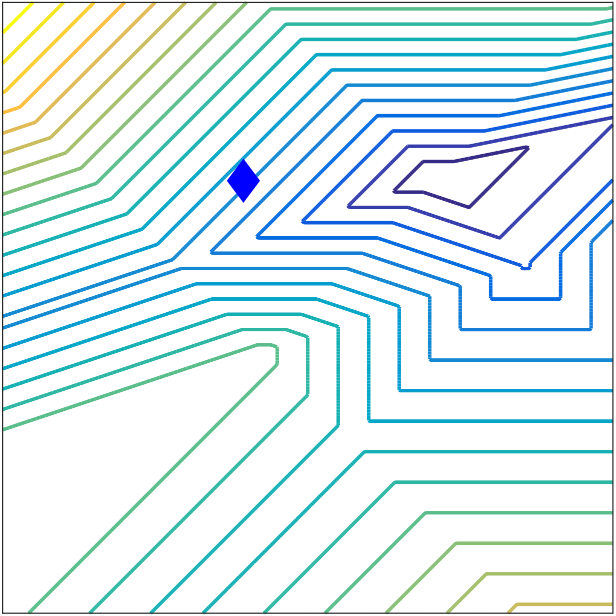

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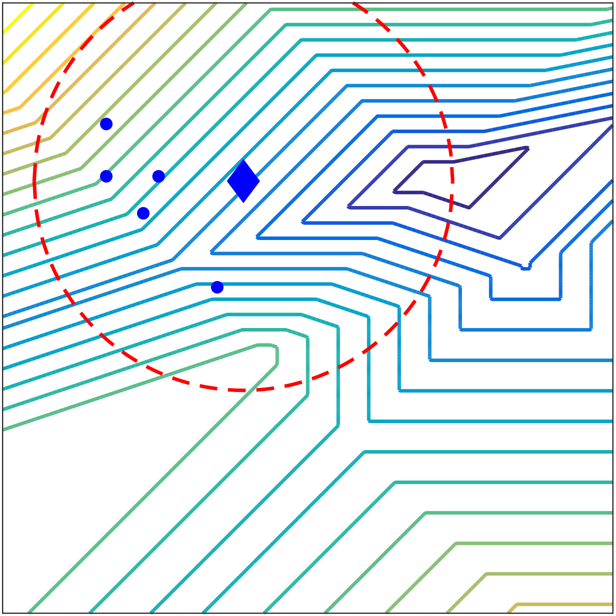

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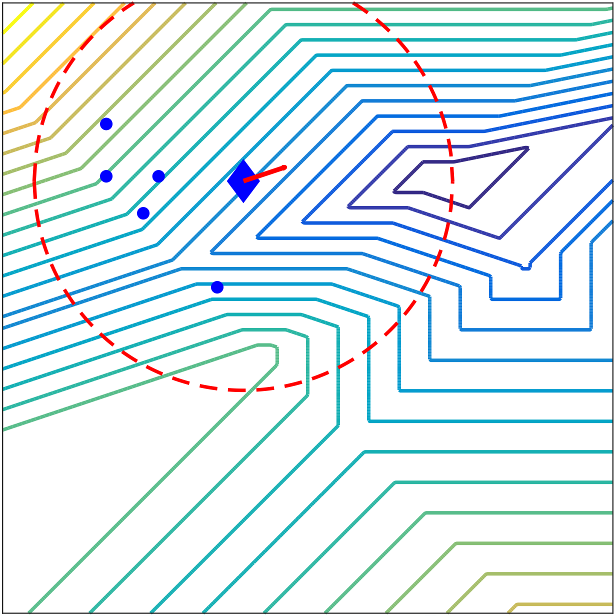
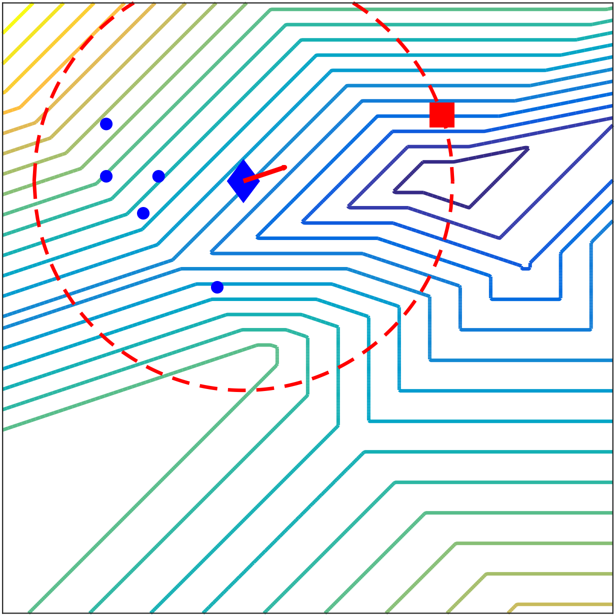


Manifold Sampling



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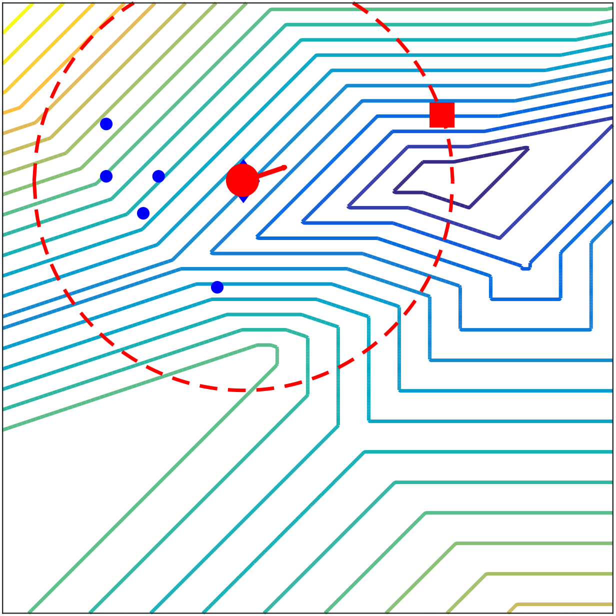

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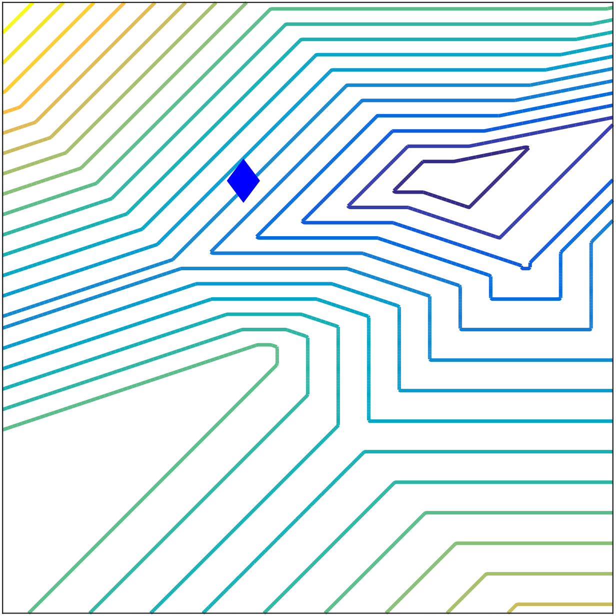

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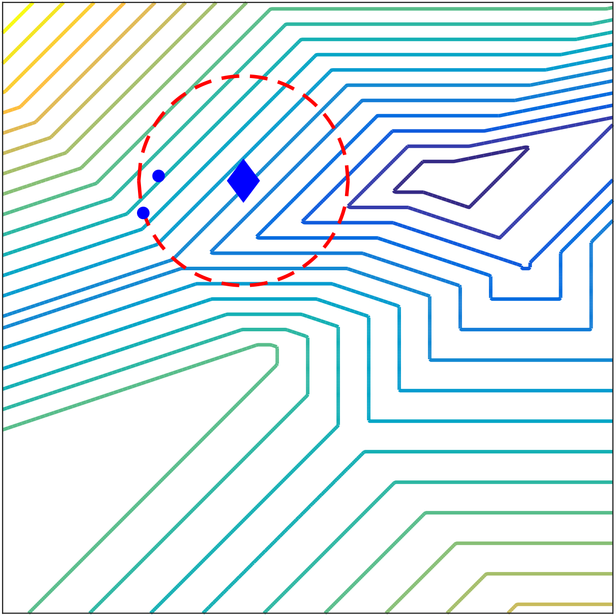

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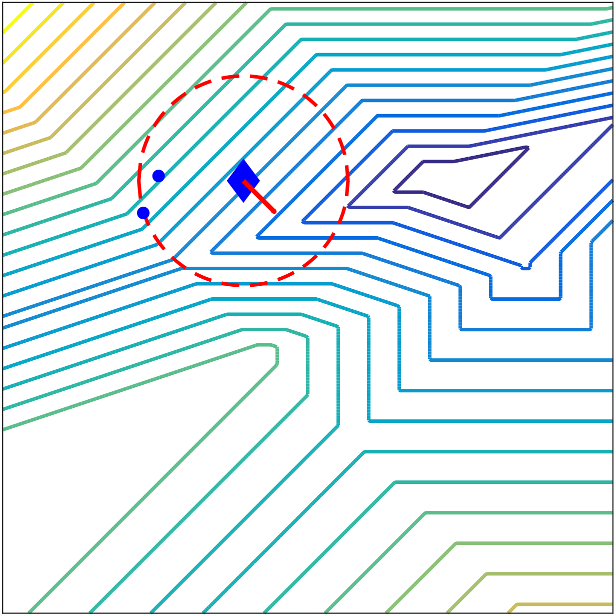

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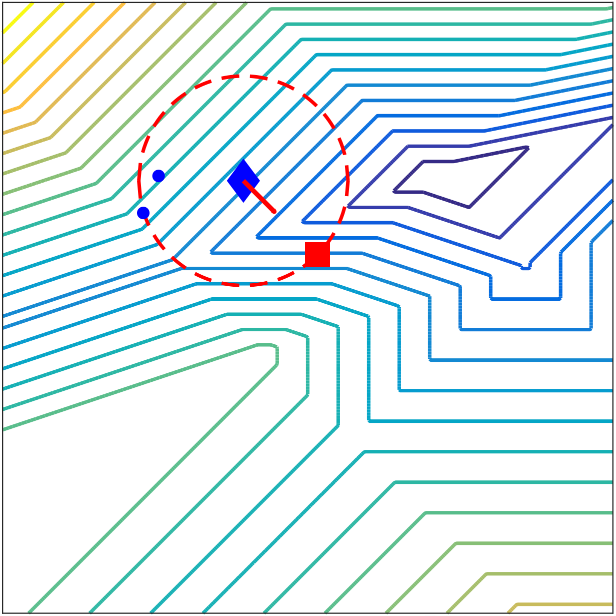

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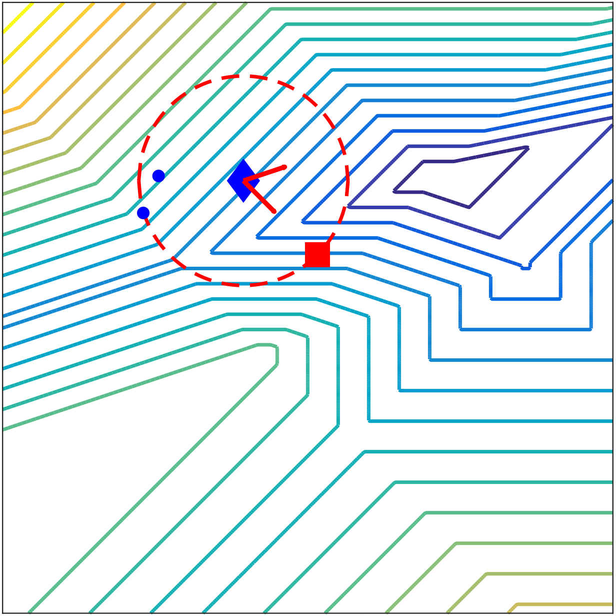

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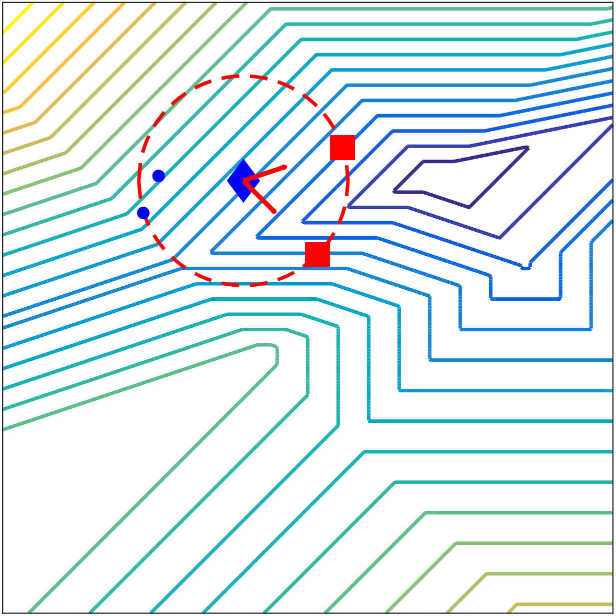

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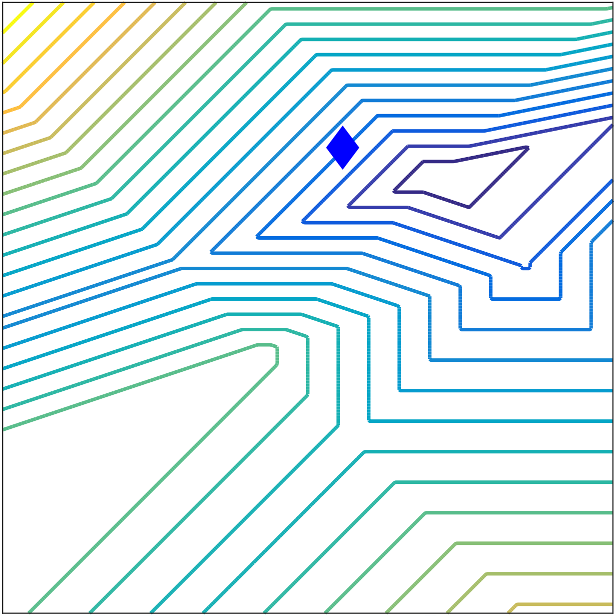

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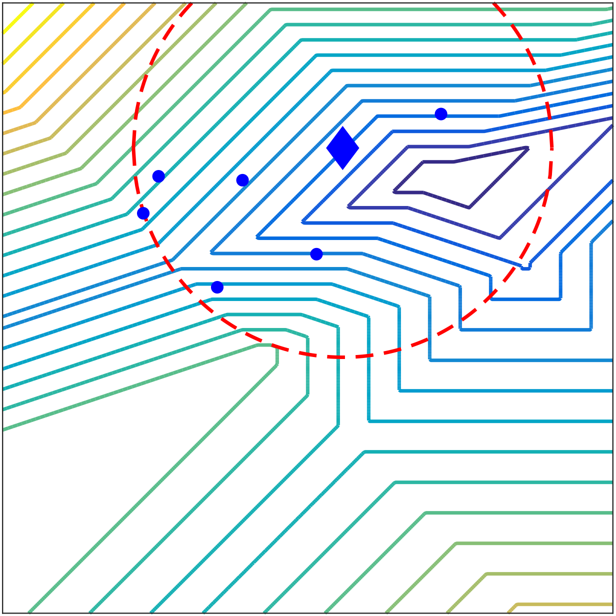

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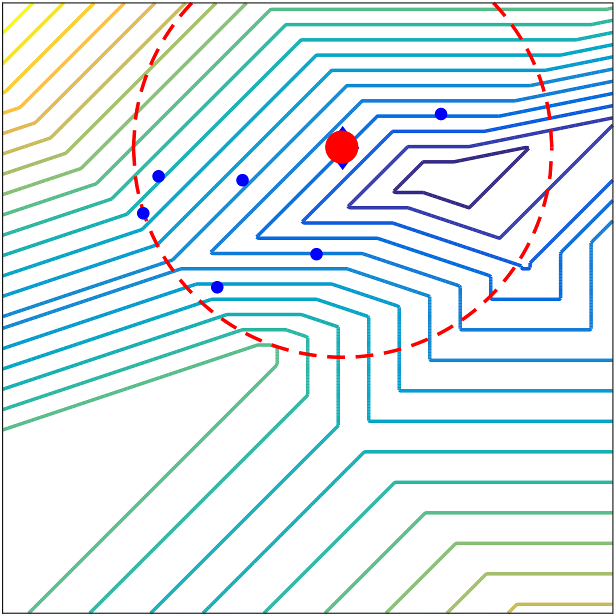

Better trust-region subproblem?

Instead of solving

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How about

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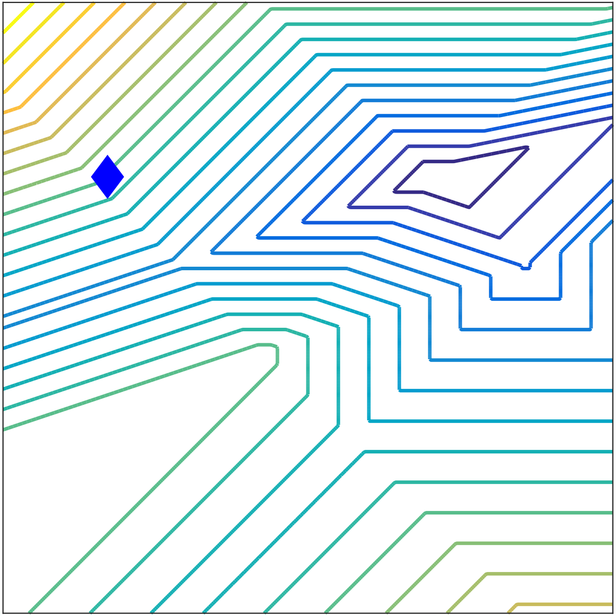

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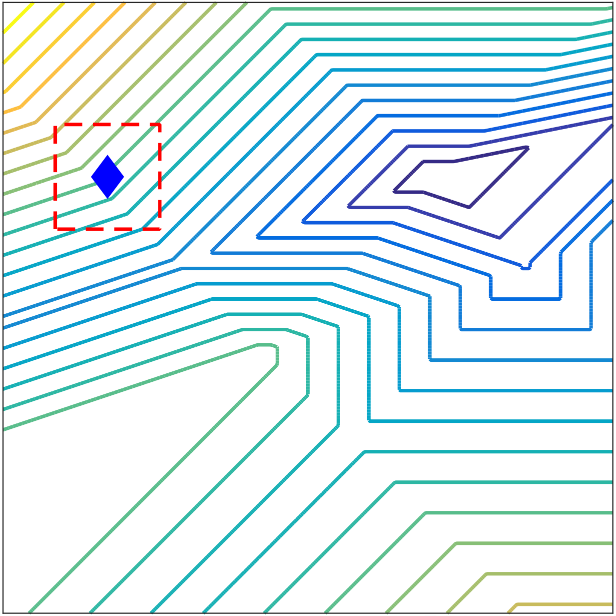

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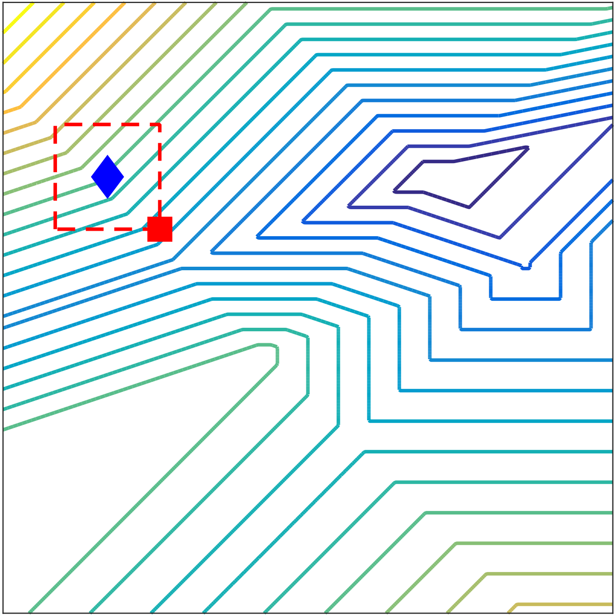

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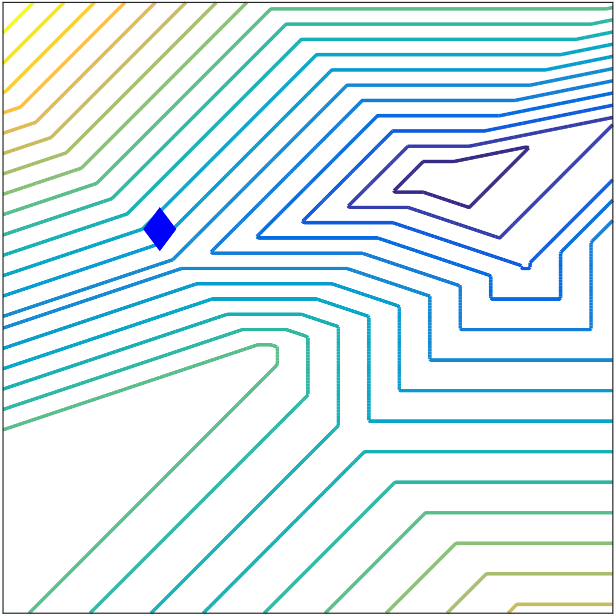

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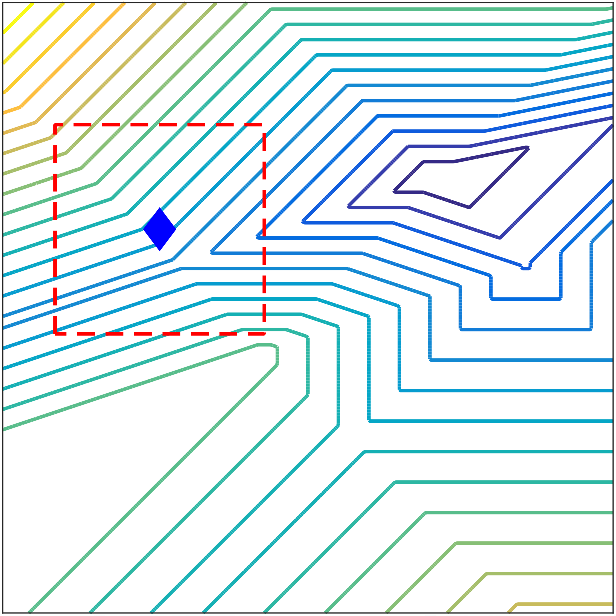

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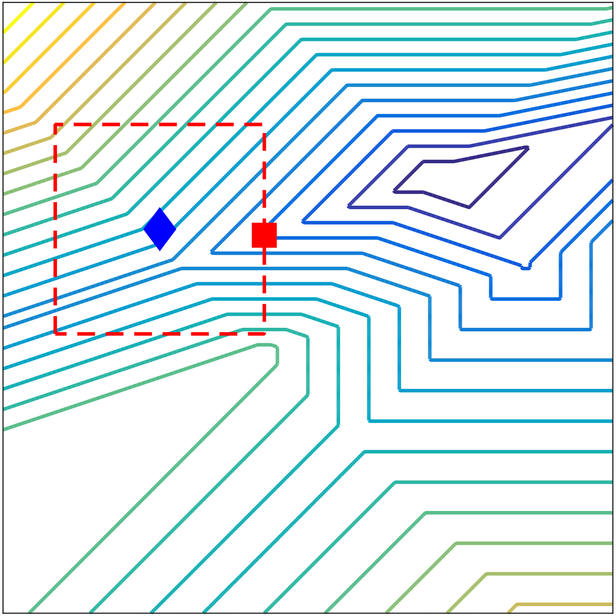

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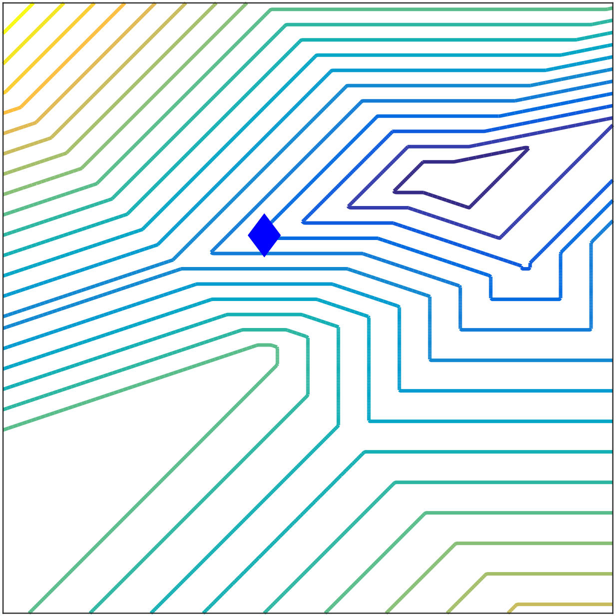

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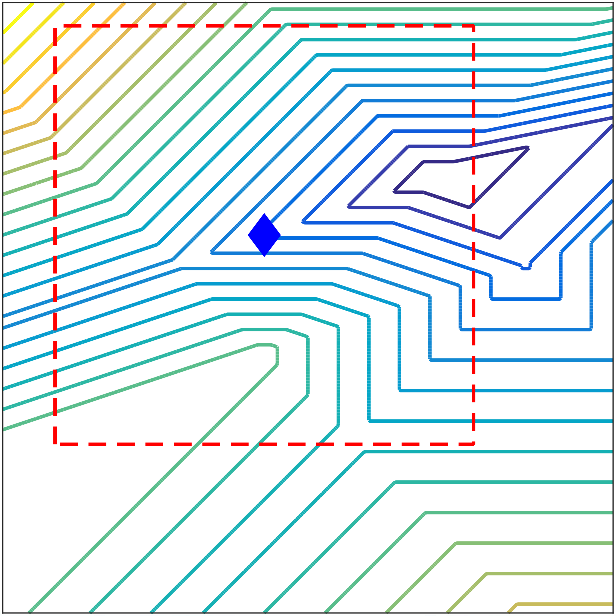

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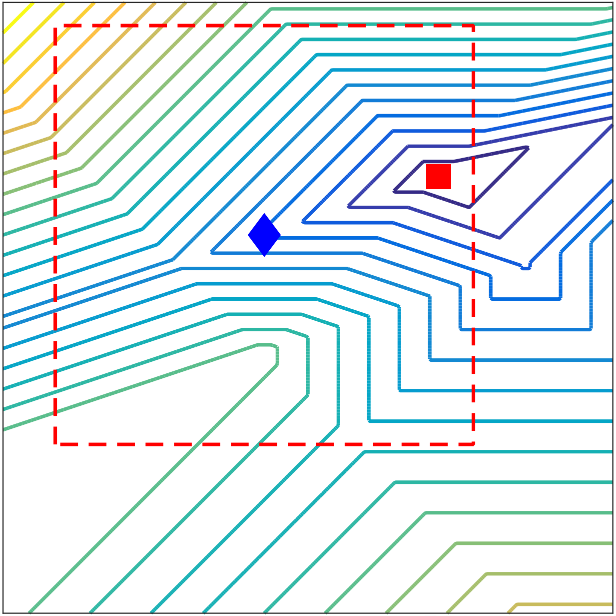

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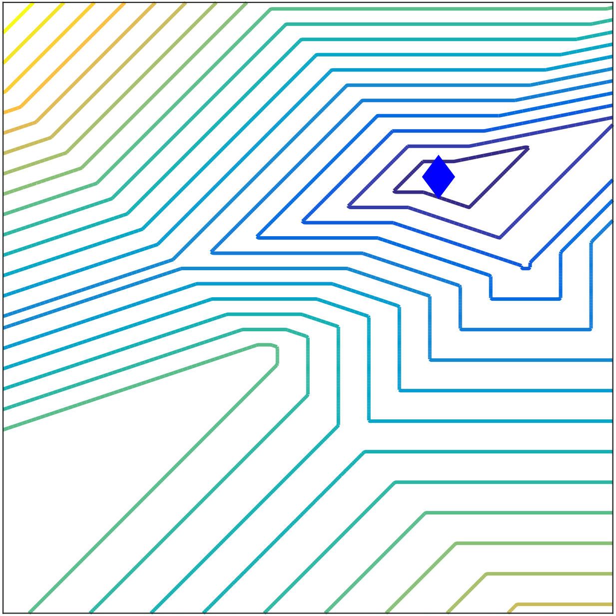

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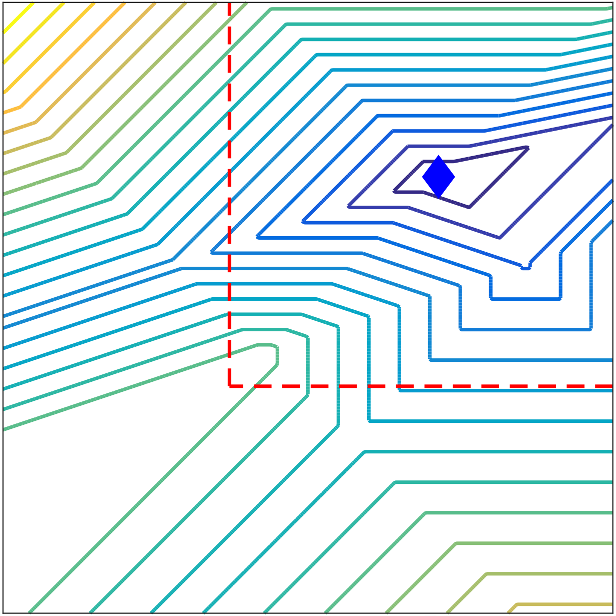

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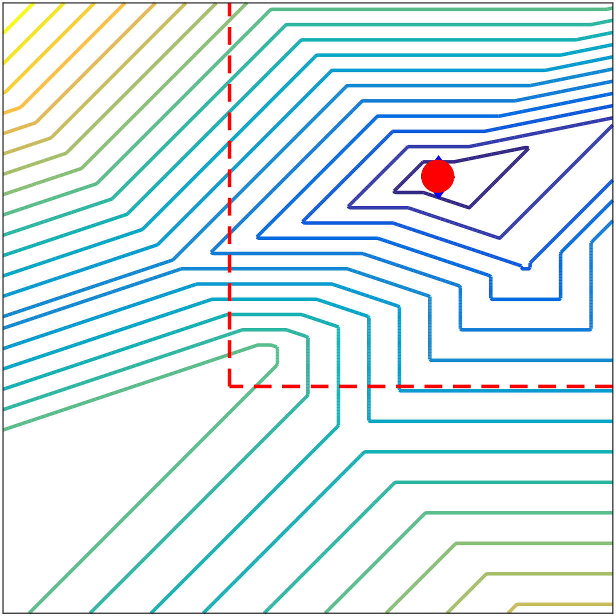

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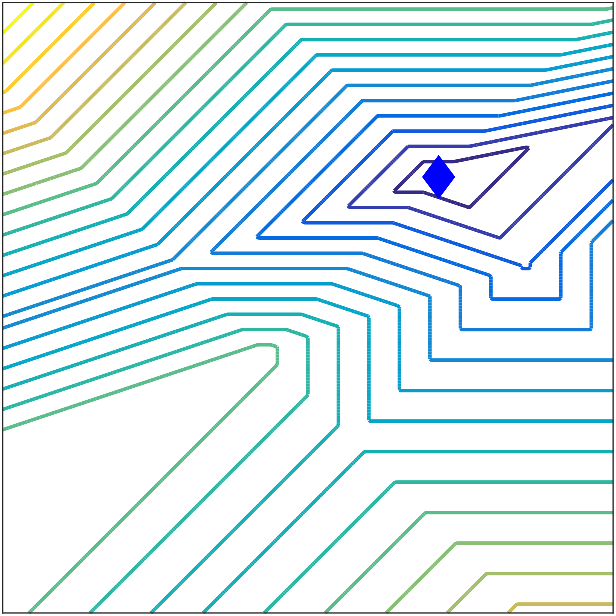

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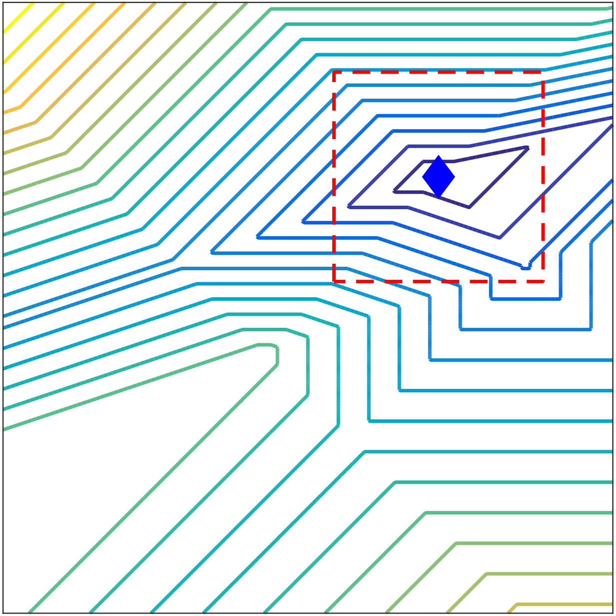

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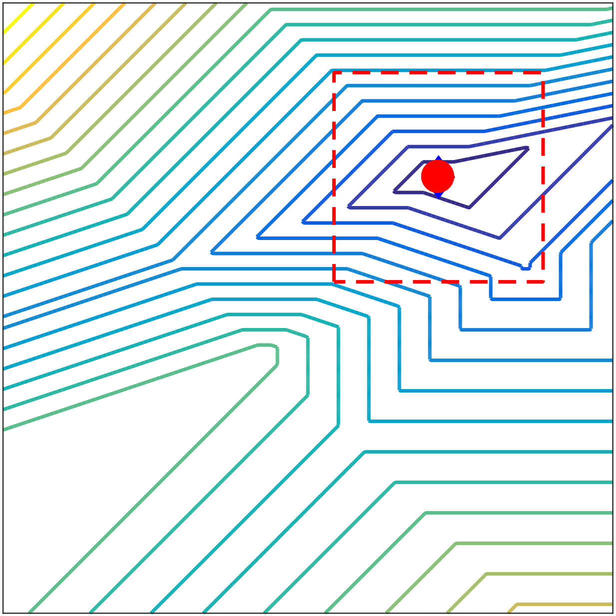

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Question

Best method for solving composite nonsmooth quadratic problems?

Thanks

Questions?

`jmlarson@anl.gov`